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AN INTRODUCTION TO DESIGN OPTIMALITY WITH AN OVERVIEW OF THE LI--ETC(U)

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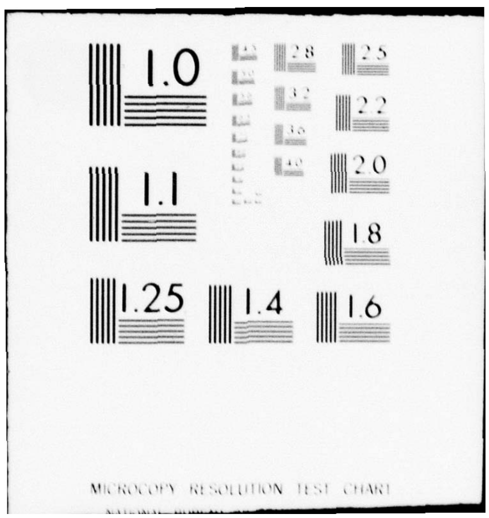
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6 An introduction to Design Optimality with an overview of the literature

by

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AN INTRODUCTION TO DESIGN OPTIMALITY
WITH AN OVERVIEW OF THE LITERATURE

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Key Words and Phrases: design; exact design; approximate design; optimal design.

ABSTRACT

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1. INTRODUCTION

An experimenter is faced with a collection of possible conditions under which to run an experiment. N observations will be made, with the goal of clarifying the relationship between the controllable conditions of the experiment and the mean value of the experimental outcome. The set of possible conditions is called the factor space, the domain, or the domain of interest. A specification for each point x in the domain as to how many n_x or equivalently what fraction p_x of the observations are to be taken at x is called a design. Sometimes there are certain restraints on how the

observations can be allocated (e.g., no more than k_x of them can be run under condition x). The collection of all allocations which meet these restraints is called the design setting. For a design to be implementable $n_x = Np_x$ must be an integer. Any design with this feature is called an exact design (with N observations). From a theoretical point of view, there are advantages to be gained from considering a broader class of designs, where N is no longer explicitly present, given as probability measures on the domain of interest. Formally, we define an approximate design, ξ, to be any probability measure on the domain. It turns out that we may restrict our attention to discrete measures ξ with support on a small number of points. For such measures and reasonably large N, an approximate design ξ is closely approximated by an exact design with N observations where each n_x is taken as an integer close to Np_x. It is known that exact designs which are thus close to best approximate designs have only slightly reduced optimality performance.

For fixed assumptions about the underlying situation, the variability associated with any estimates that are made depends only on the design. Best designs are those which in some sense minimize the errors associated with making the set of estimates which is the goal of the experiment. Since we cannot expect to simultaneously minimize all errors, we may decide, for instance, to minimize the worst expected error or, perhaps, the average expected error. Which of these is more appropriate depends on the experimental situation. There is no hope for a canonical notion of design optimality. In Section 2, we present and briefly discuss several of the most common criteria of optimality.

Throughout we are assuming that a random variable y, called the response variable, is related to a controllable variable x by a relation of the form

$$E(y|x) = f(x), \text{ or}$$

$$y|x = f(x) + \varepsilon_x, \text{ where } E(\varepsilon_x) = 0.$$

That is, the observed value of y when an experiment is run under conditions set at x is a random variable $y|x$ whose expectation is functionally related to x. The function f may be called the <u>response surface</u>, the <u>response function</u> or the <u>regression function</u>. Usually we assume that f is partially known; say $f(x) = f(x;\theta)$, where θ is a vector of unknown parameters whose specification would completely determine f.

Choosing a model means accepting the hypothesis that f has a certain functional form and that the set of errors for distinct runs of the experiment has a given covariance matrix. A <u>linear model</u> postulates that f is linear in the components of θ: $f(x,\theta) = \sum_{j=1}^{k} f_j(x)\theta_j$, although the functions f_j may well be nonlinear. When we also take V, the covariance matrix for the errors, to be of the form $\sigma^2 I_N$ we call this the <u>standard linear model</u>.

Some results are available for nonlinear models. A review of this literature can be found in St. John and Draper (1975), Section 4. If V is not $\sigma^2 I_N$, but is known, then the Y variables can be transformed to a set $Z = V^{-1/2}Y$ whose error covariance matrix is the identity. In a similar way, variable cost associated with running the experiment under different conditions x can be incorporated into the design problem through a weighting factor, $\lambda(x)$, called the *efficiency of the experiment* at x. (See, for example, Fedorov (1972), Section 1.5). Other techniques for dealing with the presence of correlated errors in regression problems have been developed by Sacks and Ylvisker (1966, 1968).

Sometimes the apparent existence of correlated errors can be practically resolved by introducing additional parameters into the response model; e.g., by postulating the existence of residual effects in situations where repeated measurements are taken on the same individual. [See Hedayat and Afsarinejad (1975, 1978) for this topic and related references].

Most of the literature concerns the standard linear model. We discuss that situation in the next section, but close in this one with an important preliminary consideration: the choice of model. Atkinson and Fedorov (1974, 1975) have discussed designs for distinguishing between rival models, but in general the problem of optimal designs to aid in such model building remains open. Work is needed to develop methodologies and measures of a methodology's effectiveness in enabling a researcher to arrive at a model through experimentation.

The problem becomes slightly more tractable if we have a model which we believe is adequate, but we are not entirely sure of it. We would like a design which simultaneously provides accurate estimates under our assumed model while providing for protection against model inadequacy. The better the design for one purpose, the worse it is for the other. Box and Draper (1959) initiated discussion of this problem in a regression setting where a polynomial function of fixed degree is fitted although the true response function is a polynomial of higher degree. Essentially, they seek designs which minimize integrated mean square error over the domain of the response function. Further work on this topic has been done, for example, by Karson, Manson and Hader (1969) and Kiefer (1973). A nice review of the work prior to 1971 is given in Stigler (1971).

Another approach has been taken by Srivastava (1975) and Srivastava and Ghosh (1977) in the fractional factorial setting, where they have found families of designs with optimality properties for the assumed model which simultaneously allow investigators to "search" for one or more parameters which should have been included in the model.

2. DESIGN OPTIMALITY FOR THE STANDARD LINEAR MODEL

We assume that $f(x) = (f_1(x),\ldots,f_k(x))'$ is a known function and $\theta = (\theta_1,\ldots,\theta_k)'$ a vector of unknown parameters such that

$$y|x = \Sigma f_j(x)\theta_j + \varepsilon_x,\ E(\varepsilon_x) = 0,\ \mathrm{Var}(\varepsilon_x) = 0,$$

and the covariances between ε_x's for distinct runs are all 0.

Our primary interest may center on either of two types of goals: estimation of some subset (perhaps all) of the parameters $\{\theta_j\}$, or estimation of the response function on some region, usually the domain of allowable x's for the design setting. (When the region of estimation contains points outside this domain, the problem becomes one of extrapolation.)

The pioneering work of Smith in 1918 introduced a first formal definition of design optimality. It was a response function criterion. Essentially, if $\hat{f}(x)$ is our estimate for $f(x)$, she constructed designs which minimized max var $\hat{f}(x)$ for x in the region of definition. Kiefer has called designs with this property G-optimal (for generalized variance); Fedorov calls them minimax. Another measure of design goodness in the presence of possible bias is integrated mean squared error, as introduced by Box and Draper (1959), although this criterion has its problems, as Kiefer points out (1973). Papers by G. E. P. Box and colleagues provide more recent references for design optimality questions oriented toward response function estimation.

Almost all of the literature on design optimality, however, has concerned criteria which are more directly related to parameter estimation. Wald's inaugural paper in this area (1943) still makes good introductory reading. Kiefer's 1974 "Lectures on Design Theory" provides a more recent, excellent overview.

If θ is estimable, then so is f, and a best linear unbiased estimate for θ is

$$\hat{\theta} = (X'X)^{-1}X'Y,$$

where X is the N×k matrix whose i^{th} row is $f(x_i)'$, the value of f at the x used in running the i^{th} experiment. Then X'X is called the information matrix of the design, and $\sigma^2(X'X)^{-1}$ is the k×k covariance matrix for the estimate $\hat{\theta}$. In some settings we may not be interested in estimating all the unknown parameters; in others, it may not even be possible to do so. In general, however, we will assume that $(\theta_1,\ldots,\theta_k)$, the unknown vector of interest, is a possibly restricted or transformed subset of the original set of unknown

parameters which is estimable, and we will designate the covariance matrix for the best linear unbiased estimator for θ as $M^{-1}\sigma^2$, where M is the information matrix of the design (for the possibly restricted parameter set θ). When we wish to emphasize M's dependence on the design d, we will write it as M(d).

It is natural to want to call a design d "optimal" when the matrix $M(d)^{-1}$ is as small as possible. The most common measures of the size of a matrix have generated the most popular measures of a design's goodness. Thus we say a design d* is D-, A- or E-optimal, if (respectively) the determinant, trace or modulus of the largest eigenvalue of M^{-1} is minimized at d*. ("A-" stands for average, since $\frac{1}{k}$ trace (M^{-1}) = average variance among $(\hat{\theta}_1, \ldots, \hat{\theta}_k)$.) Linear functionals L, defined and non-negative on the k×k non-negative definite matrices, can also be used to define plausible alternative criteria (see Fedorov (1972), Section 2.9). Best designs of this type are called L-optimal.

The Kiefer-Wolfowitz equivalence theorem (1960) has bridged the apparent gap between considerations of design optimality based on parameters versus response surface considerations. It shows that if ξ is an approximate design (a probability measure), then ξ is D-optimal $\leftrightarrow$ G-optimal $\leftrightarrow \frac{N}{\sigma^2}$ max var $\widehat{f(x)} = k$, the number of unknown parameters being estimated. The third criterion provides a valuable tool for checking that a design is D- or G-optimal, as well as for developing algorithms for construction of such designs [see, for example, Atwood (1973, 1976); Wynn (1970, 1972, 1973)].

In (1975) Kiefer introduced a "minimal" set of properties which any optimality functional, ϕ, on the k×k non-negative definite matrices should have. Roughly, we call such a function ϕ an optimality functional if (1) it is convex; (2) $\phi(cM)$ decreases as positive c increases; and (3) ϕ is insensitive to a relabelling of the unknown parameters. This broad class contains all the above optimality functionals. A design d* is said to be universally optimal if $\phi(M(d)^{-1})$ is minimized at d* for every optimality functional ϕ. Although many of the classical designs

can be shown to be universally optimal, perhaps surprisingly this is not always true for all such highly balanced structures [see, for example, Kiefer (1975)].

3. FINAL REMARKS AND PREFACE TO THE BIBLIOGRAPHY

Limitations of space and time, exacerabated undoubtedly by ignorance, have caused many interesting and important lines of research to be treated here too lightly or not at all. What we have attempted is to offer a kind of smorgasbord in which you can find a taste of each of the kinds of problems that arise in design optimality. The bibliography that follows represents a more serious attempt at comprehensiveness, but still in a limited sense. We have striven to be thorough enough to ensure that any important article can be found in at most a depth-one search; i.e., through the bibliography of an article that can be found in our listing.

One entire area of research which we have neither touched on here, nor referenced in the bibliography, is that of combinatorial design. This subject concerns the construction and combinatorial properties of designs apart from considerations of statistical optimality. Those wishing to investigate this subject may want to begin with Raghavarao (1971).

As a deeper introduction to optimal design for those familiar with the theory of linear models, we recommend Kiefer (1974b); those with some knowledge of combinatorial design may also try Kiefer (1978b).

We are grateful to Fedorov for making his bibliography of Russian and Bulgarian design articles available to us. Space limitations caused us to include only a small fraction of those articles which, from their titles, appeared most relevant to this listing. Fedorov's book is the first and so far, only

attempt to pull together the rich and diverse literature in this field. It is an important basic reference. We hope that this issue of Communications will encourage some one of you to write the second book which is so clearly needed now.

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